

# Nonadiabatic Transitions for a Decaying Two-Level-System: Geometrical and Dynamical Contributions

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We study the Landau-Zener Problem for a decaying two-level-system described by a non-hermitean Hamiltonian, depending analytically on time. Use of a super-adiabatic basis allows to calculate the non-adiabatic transition probability  $P$  in the slow-sweep limit, without specifying the Hamiltonian explicitly. It is found that  $P$  consists of a “dynamical” and a “geometrical” factors. The former is determined by the complex adiabatic eigenvalues  $E_{\pm}(t)$ , only, whereas the latter solely requires the knowledge of  $\alpha_{\pm}(t)$ , the ratio of the components of each of the adiabatic eigenstates. Both factors can be split into a universal one, depending only on the complex level crossing points, and a nonuniversal one, involving the full time dependence of  $E_{\pm}(t)$ . This general result is applied to the Akulin-Schleich model where the initial upper level is damped with damping constant  $\gamma$ . For analytic power-law sweeps we find that Stückelberg oscillations of  $P$  exist for  $\gamma$  smaller than a critical value  $\gamma_c$  and disappear for  $\gamma > \gamma_c$ . A physical interpretation of this behavior will be presented by use of a damped harmonic oscillator.

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## I. INTRODUCTION

In many cases one can reduce the quantum behavior of a system to that of a two-level system (TLS), which corresponds to a (pseudo-)spin one half. The spin-down and spin-up state will be denoted by  $|1\rangle$  and  $|2\rangle$ , respectively. If the TLS is in state  $|\Psi_0\rangle$  at time  $t_0$  one obtains  $|\Psi(t)\rangle$  by solving the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle \quad (1)$$

with initial condition  $|\Psi(t_0)\rangle = |\Psi_0\rangle$ . Note, that we allow for an explicit time dependence of  $H$ . One of the quantities of particular interest is the survival probability

$$P = \lim_{t \rightarrow \infty} \lim_{t_0 \rightarrow -\infty} |\langle \Psi(t_0) | \Psi(t) \rangle|^2 \quad (2)$$

that the system remains in its initial state. For a TLS with a level spacing depending linearly on time the result for  $P$  as function of the sweep rate  $v$  has been derived approximately by Landau [1] and Stückelberg [2] and rigorously by Zener [3] and Majorana [4].  $P$  will depend sensitively on the  $t$ -dependence of  $H$  and can not be calculated analytically, except in limiting cases, only. One of them is the adiabatic limit. In that limit it is known that  $|\Psi(t)\rangle$  converges to a superposition of the adiabatic states  $|u_{0,\pm}(t)\rangle$  which are solutions of the eigenvalue equation:

$$H(t) |u_{0,\pm}(t)\rangle = E_{\pm}(t) |u_{0,\pm}(t)\rangle \quad (3)$$

with  $E_{\pm}(t)$  the adiabatic eigenvalues. Although  $E_+(t)$  and  $E_-(t)$  may not cross in real time (avoided level-crossing) this will happen for complex times  $t_c^k$ ,  $k = 1, 2, \dots, N$ .

In case of a *real-symmetric* Hamiltonian matrix  $\langle \nu | H(t) | \nu' \rangle$ ,  $\nu, \nu' = 1, 2$  which is analytic in  $t$  and for a single crossing point  $t_c$  in the upper complex  $t$ -plane ( $\text{Im} t_c > 0$ ) it was shown by Dykhne [5] (see also earlier work by Pokrovskii et al. [6]) that

$$P \cong \exp[-2 \text{Im} z(t_c)] \quad (4)$$

in the adiabatic limit. The new variable  $z(t)$  is given by

$$z(t) = \int_0^t dt' [E_+(t') - E_-(t')]. \quad (5)$$

Davis and Pechukas [7] have performed an exact proof of result (4), (5). Particularly, these authors have proven that the pre-exponential factor equals one. Therefore it is sometimes called the Dykhne-Davis-Pechukas (DDP) formula. For more than one crossing point with  $\text{Im} z_c^k = \text{Im} z(t_c^k) > 0$  a generalization of (4) has been suggested [7, 8] and tested by Suominen and co-workers (Ref. [9] and references where-in). A rigorous prove of the generalization of DDP-formula including even *hermitean* Hamiltonians has been provided by Joye et al. [10]. More than one crossing point leads to interferences which generate oscillations in  $P$  as function of control parameters, like the sweeping rate (see below).

For Hamiltonian matrices which are not real-symmetric, but hermitean, Berry [11] and Joye et al. [12] made an interesting observation which is that  $P$  obtains also a “geometrical” factor besides the “dynamical” one, Eq. (4), where the former also depends on the crossing points  $t_c^k$ , only. For those who are less familiar with this kind of physics let us explain the choice of this nomenclature. Below we will see that one of the factors of  $P$  is entirely determined by the adiabatic eigenvalues and

the other by the adiabatic eigenstates. Since the former is important for the time evolution it is called “dynamical” whereas the latter is related to the geometry in the Hilbert space, particularly through a condition for parallel transport (Eq. 21), and accordingly it is called “geometrical”.

TLS will be influenced by their environment, e.g. by phonons. The spin-phonon coupling leads to dissipation of the (pseudo-)spin dynamics which will influence the probability  $P$ . Although there exist microscopic models for the spin-boson system [13], and simplified models where the bath is described by fluctuating fields [14, 15, 16, 17, 18], we will use a dissipative Schrödinger equation. This will be achieved by using a *non-hermitean* Hamiltonian for the TLS. A particular version of such a model has been suggested by Akulin and Schleich [19]. In their model, called AS-model in the following, the upper level (at the initial time  $t_0$ ) experiences a damping (see section III).

The survival and transition probability for non-hermitean TLS-Hamiltonians has already been investigated by Moyer [20]. This has been done by mapping the original differential equation to the Weber equation, which can be solved exactly. By use of the Weber equation as the appropriate “comparison equation” it was shown how the DDP-formula, Eqs. (4) and (5), can be extended [20]. However, this extension does not contain a “geometric” contribution, although one expects that it exists similarly to what has been proven for hermitean matrices [11, 12]. On the other hand Garrison and Wright [21] have investigated the geometrical phase for dissipative systems but not the non-adiabatic transition probability.

It is one of our main goals to derive a generalized DDP-formula in the adiabatic limit containing a “geometrical” and a “dynamical” contribution for a *general* non-hermitean TLS-Hamiltonian. We will demonstrate that both contributions consist of a universal and a non-universal part. The former depends only on the complex crossing points whereas the latter requires the knowledge of the complete time dependence of  $H$ . Instead of using a “comparison equation” we apply the concept of a *superadiabatic* basis, put forward by Berry [22], to non-hermitean TLS-Hamiltonians. As a result we will find that the “dynamical” contribution to the non-adiabatic transition probability (which equals the survival probability in the adiabatic limit) is determined by the complex, adiabatic eigenvalues  $E_{\pm}(t)$ , only. The corresponding “geometrical” part solely requires the knowledge of  $\alpha_{\pm}(t)$ , the ratio of the components of each of the *adiabatic* eigenstates.

A second motivation is the application of our results to the AS-model. It has been shown that the survival probability  $P$  does not depend on the damping coefficient  $\gamma$  of the upper level, provided the bias of the TLS varies *linearly* in time, and the coupling  $\Delta$  between both levels is time-independent [19]. Therefore it is interesting to investigate *non-linear* time dependence and to check

whether or not  $P$  remains insensitive on  $\gamma$ . For non-linear time dependence more than one complex crossing points may occur, such that interference effects can govern the dependence of  $P$  on the sweeping rate [10]. Specific examples with  $\gamma = 0$  for which this happens were discussed in recent years [9, 23]. There it was found that critical values for the sweeping rate exists at which the survival probability vanishes, i.e. complete transitions occur between both quantum levels. Consequently, one may ask: Are these complete transitions reduced or even suppressed in the presence of damping?

Our paper is organized as follows. The next section will contain the general treatment of the non-hermitean Hamiltonian and the presentation of the generalized DDP-formula. In section III we will apply the results from the second section to the AS-model with power law time dependence. The results for the AS-model for power law sweeps can be interpreted by the dynamics of a damped harmonic oscillator. This will be shown in section IV. A short summary and some conclusions are given in the final section.

## II. GENERAL FORMULA FOR NONADIABATIC TRANSITION PROBABILITY

In this section, we will derive a generalized DDP-formula for the non-adiabatic transition problem of a decaying TLS. The Hamiltonian can be represented as follows

$$H(\delta t/\hbar) = \frac{1}{2} \sum_{j=1}^3 B_j(\delta t/\hbar) \sigma_j \quad (6)$$

with  $\sigma_j$ , the Pauli-matrices and  $B_j$  a time dependent field.  $\delta > 0$  is the adiabaticity parameter. Because this model should be dissipative, at least one of the  $B_j$  must contain a nonzero imaginary part. Accordingly  $H$  is non-hermitean. In the following we will assume that  $B_j$  is analytic in  $t$ . Introducing a new time variable

$$\tau = \delta t/\hbar \quad (7)$$

Eq. (1) becomes

$$i\delta d_{\tau}|\Psi(\tau)\rangle = H(\tau)|\Psi(\tau)\rangle, \quad (8)$$

where  $d_{\tau} = \partial/\partial\tau$ .  $|\Psi(\tau)\rangle$  can be expanded with respect to  $|\nu\rangle$

$$|\Psi(\tau)\rangle = \sum_{\nu=1}^2 c_{\nu}(\tau)|\nu\rangle. \quad (9)$$

With  $|\Psi(\tau_0)\rangle$ , the initial state, its survival probability is

$$P \equiv P(\delta) = \lim_{\tau \rightarrow \infty} \lim_{\tau_0 \rightarrow -\infty} |\langle\Psi(\tau_0)|\Psi(\tau)\rangle|^2. \quad (10)$$

Note that  $P$  is the survival probability with respect to the *adiabatic* basis. With respect to the *adiabatic* basis  $P$  is the nonadiabatic transition probability.

To calculate  $P$  for  $\delta \ll 1$  we introduce the *adiabatic basis* of  $H(\tau)$ . This can be done as in Ref. [21] where a biorthonormal set of right-eigenstates was used or alternatively by use of left- and right-eigenstates. We will use the latter, as it turns out to be more elegant. Let

$$|u_{0,\pm}(\tau)\rangle = \sum_{\nu=1}^2 e_{\pm}^{\nu}(\tau)|\nu\rangle \quad (11)$$

be the adiabatic *right*-eigenstates. They are solutions of

$$H(\tau)|u_{0,\pm}(\tau)\rangle = E_{\pm}(\tau)|u_{0,\pm}(\tau)\rangle \quad (12)$$

with  $E_{\pm}(\tau)$ , the adiabatic eigenvalues. Note that  $E_{\pm}(\tau)$  are complex in general and that the norm of  $|u_{0,\pm}(\tau)\rangle$  and of  $|\Psi(\tau)\rangle$  is *not* conserved, since  $H(\tau)$  is nonhermitean. Following Berry [22], we introduce a hierarchy of *superadiabatic* right-eigenstates  $|u_{n,\pm}(\tau)\rangle$ ,  $n = 0, 1, 2, \dots$  and expand the solutions  $|\Psi_{\pm}(\tau)\rangle$  of Eq. (8) with respect to the superadiabatic basis:

$$|\Psi_{\pm}(\tau)\rangle = \exp \left[ -\frac{i}{\delta} \int_{\tau_0}^{\tau} d\tau' E_{\pm}(\tau') \right] \sum_{m=0}^{\infty} \delta^m |u_{m,\pm}(\tau)\rangle. \quad (13)$$

Substituting  $|\Psi_{\pm}(\tau)\rangle$  into Eq. (8) yields the recursion relations

$$[H(\tau) - E_{\sigma}(\tau)]|u_{0,\sigma}(\tau)\rangle = 0, \quad \sigma = \pm \quad (14)$$

$$i d_{\tau} |u_{m-1,\sigma}(\tau)\rangle = [H(\tau) - E_{\sigma}(\tau)]|u_{m,\sigma}(\tau)\rangle, \quad m \geq 1. \quad (15)$$

Eq. (14) is already fulfilled, due to Eq. (12). To make progress we introduce the adiabatic *left*-eigenstates

$$\langle \tilde{u}_{0,\sigma}(\tau) | = \sum_{\nu=1}^2 \tilde{e}_{\sigma}^{\nu}(\tau) \langle \nu | \quad (16)$$

which are solutions of

$$\langle \tilde{u}_{0,\sigma}(\tau) | H(\tau) = E_{\sigma}(\tau) \langle \tilde{u}_{0,\sigma}(\tau) | \quad (17)$$

and are normalized such that:

$$\langle \tilde{u}_{0,\sigma}(\tau) | u_{0,\sigma'}(\tau) \rangle = \delta_{\sigma\sigma'}. \quad (18)$$

Let be:

$$\alpha_{\sigma}(\tau) = \frac{e_{\sigma}^2(\tau)}{e_{\sigma}^1(\tau)}, \quad (19)$$

the ratio of the components of the adiabatic right-eigenstate  $|u_{0,\sigma}(\tau)\rangle$ . Then it is straightforward to prove that

$$\tilde{e}_{\sigma}^{\nu}(\tau) = \frac{\sigma}{[\alpha_{+}(\tau) - \alpha_{-}(\tau)]e_{\sigma}^1(\tau)} \begin{cases} -\alpha_{\mp}(\tau), & \nu = 1 \\ 1, & \nu = 2 \end{cases} \quad (20)$$

which defines the left-eigenstate from the right-eigenstate. Multiplication of Eq. (15) for  $m = 1$  with  $\langle \tilde{u}_{0,\sigma}(\tau) |$  leads to

$$\langle \tilde{u}_{0,\sigma}(\tau) | d_{\tau} | u_{0,\sigma}(\tau) \rangle \equiv 0, \quad \sigma = \pm. \quad (21)$$

This is the condition for “parallel transport” [11, 24] now generalized to nonhermitean Hamiltonians.

In order to solve recursion (15) we expand  $|u_{m,\sigma}(\tau)\rangle$ ,  $m \geq 1$  with respect to  $|u_{0,\sigma}(\tau)\rangle$ :

$$|u_{m,\sigma}(\tau)\rangle = a_m^{\sigma}(\tau)|u_{0,-}(\tau)\rangle + b_m^{\sigma}(\tau)|u_{0,+}(\tau)\rangle. \quad (22)$$

Substitution of Eq. (22) into Eq. (15) and multiplying by  $\langle \tilde{u}_{0,\sigma}(\tau) |$  yields with Eqs. (14), (18) for  $m \geq 1$ :

$$\dot{a}_{m-1}^{-}(\tau) = -\kappa_{-}(\tau)b_{m-1}(\tau) \quad (23)$$

$$\dot{b}_{m-1}^{-}(\tau) = -\kappa_{+}(\tau)a_{m-1}^{-}(\tau) - i[E_{+}(\tau) - E_{-}(\tau)]b_{m-1}^{-}(\tau), \quad (24)$$

where  $\dot{\phantom{x}}$  denotes derivative with respect to  $\tau$  and

$$\kappa_{\sigma}(\tau) = \langle \tilde{u}_{0,\sigma}(\tau) | d_{\tau} | u_{0,-\sigma}(\tau) \rangle \quad (25)$$

are the nonadiabatic coupling functions, responsible for the nonadiabatic transitions. If  $\kappa_{\sigma}(\tau) \equiv 0$ , we get from Eqs. (23) and (24)

$$a_m^{-}(\tau) \equiv a_m^{-}(\tau_0), \quad b_m^{-}(\tau) = \frac{i}{E_{+}(\tau) - E_{-}(\tau)} \dot{b}_{m-1}^{-}(\tau). \quad (26)$$

Similar equations follow for  $a_m^{+}(\tau)$ ,  $b_m^{+}(\tau)$ , which however, will not be needed. Next we fix the initial condition for  $|\Psi_{\sigma}(\tau)\rangle$ :

$$|\Psi_{\sigma}(\tau_0)\rangle = |u_{0,\sigma}(\tau_0)\rangle, \quad (27)$$

i.e., we start in the adiabatic right-eigenstates. From Eqs. (13), (22) we find immediately for  $\sigma = -$

$$a_0^{-}(\tau) \equiv 1, \quad b_0^{-}(\tau) \equiv 0 \\ a_m^{-}(\tau_0) = 0, \quad b_m^{-}(\tau_0) = 0, \quad m \geq 1. \quad (28)$$

such that Eq. (26) implies  $a_m^{-}(\tau) \equiv 0$ ,  $b_m^{-}(\tau) \equiv 0$ ,  $m \geq 1$  provided  $\kappa_{\pm}(\tau) \equiv 0$ . This makes obvious the absence of nonadiabatic transitions.

The next step is the calculation of  $\kappa_{\sigma}(\tau)$ . For this we need  $e_{\sigma}^1(\tau)$ , which can be determined from (21). As a result we find

$$e_{\sigma}^1(\tau) = e_{\sigma}^1(\tau_0) \exp \left[ -\sigma \int_{\tau_0}^{\tau} d\tau' \frac{\dot{\alpha}_{\sigma}(\tau')}{\alpha_{+}(\tau') - \alpha_{-}(\tau')} \right], \quad (29)$$

and taking Eq. (20) into account we obtain the general result

$$\kappa_{\sigma}(\tau) = \sigma \frac{e_{-\sigma}^1(\tau_0)}{e_{\sigma}^1(\tau_0)} \exp \left[ \sigma \int_{\tau_0}^0 d\tau' \frac{\dot{\alpha}_{+}(\tau') + \dot{\alpha}_{-}(\tau')}{\alpha_{+}(\tau') - \alpha_{-}(\tau')} \right] \\ \times \frac{\dot{\alpha}_{-\sigma}(\tau)}{\alpha_{+}(\tau) - \alpha_{-}(\tau)} \exp \left[ \sigma \int_0^{\tau} d\tau' \frac{\dot{\alpha}_{+}(\tau') + \dot{\alpha}_{-}(\tau')}{\alpha_{+}(\tau') - \alpha_{-}(\tau')} \right] \quad (30)$$

where the expression has been split into a  $\tau$ -independent (first line) and a  $\tau$ -dependent factor (second line). Following Berry [22] we truncate the series, Eq. (13), at the  $n$ -th level

$$|\Psi_{n,\sigma}(\tau)\rangle = \exp \left[ -\frac{i}{\delta} \int_{\tau_0}^{\tau} d\tau' E_{\sigma}(\tau') \right] \sum_{m=0}^n \delta^m |u_{m,\sigma}(\tau)\rangle. \quad (31)$$

and expand  $|\Psi(\tau)\rangle$ :

$$|\Psi(\tau)\rangle = \sum_{\sigma=\pm} c_{n,\sigma}(\tau) |\Psi_{n,\sigma}(\tau)\rangle. \quad (32)$$

As initial condition we choose:

$$|\Psi(\tau_0)\rangle = |\Psi_{-}(\tau_0)\rangle, \quad (33)$$

which is equivalent to

$$c_{n,-}(\tau_0) = 1, \quad c_{n,+}(\tau_0) = 0, \quad n \rightarrow \infty. \quad (34)$$

Introducing a corresponding truncated state

$$\langle \tilde{\Psi}_{n,\sigma}(\tau) | = f_{n,\sigma}(\tau) \sum_{m=0}^n \delta^m \langle \tilde{u}_{m,\sigma}(\tau) |, \quad (35)$$

where the  $\tau$ -dependent prefactor  $f_{n,\sigma}(\tau)$  has not to be specified we obtain an equation of motion for  $c_{n,\sigma}(\tau)$ , after Eq. (32) has been substituted into Eq. (8):

$$i\delta \dot{c}_{n,\sigma}(\tau) = \sum_{\sigma'} H_{n;\sigma\sigma'}(\tau) c_{n,\sigma'}(\tau) \quad (36)$$

with

$$\begin{aligned} H_{n;\sigma\sigma'}(\tau) &= \sum_{\sigma''=\pm} (\mathcal{L}_n^{-1}(\tau))_{\sigma\sigma''} \mathcal{H}_{n;\sigma''\sigma'}(\tau) \\ \mathcal{L}_{n;\sigma\sigma'}(\tau) &= \langle \tilde{\Psi}_{n,\sigma}(\tau) | \Psi_{n,\sigma'}(\tau) \rangle \\ \mathcal{H}_{n;\sigma\sigma'}(\tau) &= \langle \tilde{\Psi}_{n,\sigma}(\tau) | H(\tau) - i\delta d_{\tau} | \Psi_{n,\sigma'}(\tau) \rangle. \end{aligned} \quad (37)$$

Eq. (36) can be rewritten as an integral equation

$$\begin{aligned} c_{n,\sigma}(\tau) &= c_{n,\sigma}(\tau_0) + \frac{i}{\delta} \int_{\tau_0}^{\tau} d\tau' H_{n;\sigma,-\sigma}(\tau') c_{n,-\sigma}(\tau') \\ &\times \exp \left[ -\frac{i}{\delta} \int_{\tau'}^{\tau} d\tau'' H_{n;\sigma\sigma}(\tau'') \right]. \end{aligned} \quad (38)$$

Apart from the truncation, Eq. (31), the results are still exact. Eq. (38) simplifies in the adiabatic limit  $\delta \rightarrow 0$ . In leading order in  $\delta$  we get from Eqs. (18), (31) and (35)

$$\mathcal{L}_{n;\sigma\sigma'}(\tau) \cong f_{n,\sigma}(\tau) \exp \left[ -\frac{i}{\delta} \int_{\tau_0}^{\tau} d\tau' E_{\sigma}(\tau') \right] \delta_{\sigma\sigma'} \quad (39)$$

$[H(\tau) - i\delta d_{\tau}] |\Psi_{n,\sigma'}(\tau)\rangle$  can be found in Ref. [21]. Multiplying by  $\langle \tilde{\Psi}_{n,\sigma}(\tau) |$  and making use of Eqs. (12), (18), (22) and (35) leads to

$$\begin{aligned} \mathcal{H}_{n;\sigma\sigma'}(\tau) &= -\delta^{n+1} f_{n,\sigma}(\tau) [E_{\sigma}(\tau) - E_{\sigma'}(\tau')] \\ &\times \exp \left[ -\frac{i}{\delta} \int_{\tau_0}^{\tau} d\tau' E_{\sigma'}(\tau') \right] \\ &\times \left[ a_{n+1}^{\sigma'}(\tau) \delta_{\sigma,-} + b_{n+1}^{\sigma'}(\tau) \delta_{\sigma,+} \right] + \mathcal{O}(\delta^{n+2}) \end{aligned} \quad (40)$$

from which follows

$$\begin{aligned} H_{n;\sigma\sigma'}(\tau) &= -\delta^{n+1} \left[ a_{n+1}^{\sigma'}(\tau) \delta_{\sigma,-} + b_{n+1}^{\sigma'}(\tau) \delta_{\sigma,+} \right] \\ &\times [E_{\sigma}(\tau) - E_{\sigma'}(\tau)] \\ &\times \exp \left\{ \frac{i}{\delta} \int_{\tau_0}^{\tau} d\tau' [E_{\sigma}(\tau') - E_{\sigma'}(\tau')] \right\} + \mathcal{O}(\delta^{n+2}) \end{aligned} \quad (41)$$

Note that the prefactor  $f_{n,\sigma}(\tau)$  has cancelled. The diagonal elements of  $\mathbf{H}_n(\tau)$  are of order  $\delta^{n+2}$  and the non-diagonal ones of order  $\delta^{n+1}$ . Therefore it follows from Eqs. (23), (30), (34) and (38)

$$\begin{aligned} c_{n,+}(\tau) &\cong i\delta^n \frac{e_{-}^1(\tau_0)}{e_{+}^1(\tau_0)} \exp \left[ \int_{\tau_0}^0 d\tau' \frac{\dot{\alpha}_{+}(\tau') + \dot{\alpha}_{-}(\tau')}{\alpha_{+}(\tau') - \alpha_{-}(\tau')} \right] \\ &\times \int_{\tau_0}^{\tau} d\tau' \dot{\alpha}_{n+1}^{-}(\tau') \frac{[\alpha_{+}(\tau') - \alpha_{-}(\tau')]}{\dot{\alpha}_{+}(\tau')} [E_{+}(\tau') - E_{-}(\tau')]. \\ &\times \exp \left[ \int_0^{\tau'} d\tau'' \frac{\dot{\alpha}_{+}(\tau'') + \dot{\alpha}_{-}(\tau'')}{\alpha_{+}(\tau'') - \alpha_{-}(\tau'')} \right] \\ &\times \exp \left\{ \frac{i}{\delta} \int_{\tau_0}^{\tau'} d\tau'' [E_{+}(\tau'') - E_{-}(\tau'')] \right\}. \end{aligned} \quad (42)$$

The time dependence of  $H(\tau)$  is chosen such that

$$\begin{aligned} \lim_{\tau_0 \rightarrow -\infty} |u_{0,-}(\tau_0)\rangle &= |1\rangle, \quad \lim_{\tau_0 \rightarrow -\infty} |u_{0,+}(\tau_0)\rangle = |2\rangle \\ \lim_{\tau \rightarrow \infty} |u_{0,-}(\tau)\rangle &\sim |2\rangle, \quad \lim_{\tau \rightarrow \infty} |u_{0,+}(\tau)\rangle \sim |1\rangle. \end{aligned} \quad (43)$$

Note that the adiabatic states at initial time  $\tau_0$  are normalized. Since Eqs. (27), (33) and (43) imply

$$\lim_{\tau_0 \rightarrow -\infty} |\Psi(\tau_0)\rangle = |1\rangle \quad (44)$$

we obtain from Eq. (10) for the nonadiabatic transition probability in leading order in  $\delta$

$$P(\delta) \cong \left| c_{n,+}(\infty) \langle 1 | u_{0,+}(\infty) \rangle \exp \left[ -\frac{i}{\delta} \int_{-\infty}^{\infty} d\tau' E_{+}(\tau') \right] \right|^2, \quad (45)$$

where we used  $\langle 1|u_{0,-}(\infty)\rangle = 0$ , due to Eq. (43). Substituting  $c_{n,+}(\infty)$  from Eq. (42) with  $\tau_0 = -\infty$  into Eq. (45) we get with Eqs. (11), (29) and  $\lim_{\tau_0 \rightarrow -\infty} e_-^1(\tau_0) = 1$  (due to Eq. (43))

$$\begin{aligned}
P(\delta) &\cong \exp \left[ -\left( F_g^{ns} + \frac{1}{\delta} F_d^{ns} \right) \right] \\
&\times \left| \delta^n \int_{-\infty}^{\infty} d\tau \dot{\alpha}_{n+1}^-(\tau) \frac{\alpha_+(\tau) - \alpha_-(\tau)}{\dot{\alpha}_+(\tau)} [E_+(\tau) - E_-(\tau)] \right. \\
&\times \exp \left[ \int_0^{\tau} d\tau' \frac{\dot{\alpha}_+(\tau') + \dot{\alpha}_-(\tau')}{\alpha_+(\tau') - \alpha_-(\tau')} \right] \\
&\times \exp \left\{ \frac{i}{\delta} \int_0^{\tau} d\tau' [E_+(\tau') - E_-(\tau')] \right\} \Bigg|^2 \quad (46)
\end{aligned}$$

with the *nonsingular* “geometrical” and “dynamical” contribution

$$\begin{aligned}
F_g^{ns} &= 2\text{Re} \left[ \int_0^{\infty} d\tau \frac{\dot{\alpha}_+(\tau)}{\alpha_+(\tau) - \alpha_-(\tau)} \right. \\
&\quad \left. - \int_{-\infty}^0 d\tau \frac{\dot{\alpha}_-(\tau)}{\alpha_+(\tau) - \alpha_-(\tau)} \right] \quad (47)
\end{aligned}$$

and

$$F_d^{ns} = -2\text{Im} \left[ \int_0^{\infty} d\tau E_+(\tau) + \int_{-\infty}^0 d\tau E_-(\tau) \right], \quad (48)$$

respectively. Note that  $F_d^{ns} = 0$ , for a hermitean Hamiltonian, since  $E_{\sigma}(\tau)$  are real. The expressions for  $F_g^{ns}$  and  $F_d^{ns}$  put some constraints on  $H(\tau)$ , because both quantities should be larger or equal to a constant  $c > -\infty$ , which requires that  $\text{Im}E_{\pm}(\tau)$  decays fast enough for  $\tau \rightarrow \pm\infty$ .

The  $\tau$ -integral in Eq. (46) is dominated by the singularities of  $E_+(\tau) - E_-(\tau)$ , for  $\delta \rightarrow 0$ . The adiabatic eigenvalues and  $\alpha_{\pm}(\tau)$  have the form

$$E_{\pm}(\tau) = \frac{1}{2} \left[ T(\tau) \pm \sqrt{T^2(\tau) - 4D(\tau)} \right] \quad (49)$$

$$\alpha_{\pm}(\tau) = \frac{-H_{11}(\tau) + H_{22}(\tau) \pm \sqrt{T^2(\tau) - 4D(\tau)}}{2H_{12}(\tau)}, \quad (50)$$

where  $T$  and  $D$ , is respectively, the trace and the determinant of the Hamiltonian matrix  $H_{\nu\nu'} = \langle \nu | H | \nu' \rangle$ . Accordingly, the singularities are the branch points  $\tau_c(k)$ ,  $k = 1, 2, \dots$  of  $E_+(\tau) - E_-(\tau)$ . Introducing a new variable [10, 22]

$$z(\tau) = \int_0^{\tau} d\tau' [E_+(\tau') - E_-(\tau')] \quad (51)$$

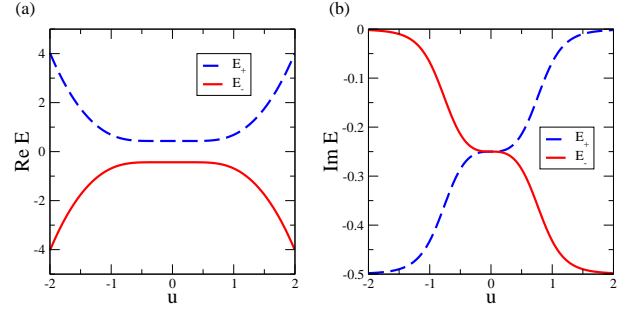


FIG. 1:  $u$ -dependence of the adiabatic eigenvalues for a power law sweep  $\tilde{w}(u) = u^3$  and  $\tilde{\gamma} = 0.5 < \tilde{\gamma}_c = 1$  (a) real part of  $E_{\pm}(u)$ , and (b) imaginary part of  $E_{\pm}(u)$

it is shown in the Appendix A that after taking the limit  $n \rightarrow \infty$  the nonadiabatic transition probability is given by

$$P(\delta) \cong \exp \left[ -\left( F_g^{ns} + \frac{1}{\delta} F_d^{ns} \right) \right] \left| \sum_k \exp F_g^s(k) e^{\frac{i}{\delta} z_c(k)} \right|^2 \quad (52)$$

with the *singular* “geometrical” contribution

$$F_g^s(k) = \int_0^{z_c(k)} dz \frac{\frac{d\alpha_+}{dz}(z) - \frac{d\alpha_-}{dz}(z)}{\alpha_+(z) - \alpha_-(z)} \quad (53)$$

and the singular points  $z_c(k) = z(\tau_c(k))$ , which are *above* the contour  $\mathcal{C} = \{z(\tau) | -\infty \leq \tau \leq \infty\}$ . The final result of this section, Eq. (52), is the generalization of the DDP formula (as it has been rigorously proven for hermitean TLS-Hamiltonians [10]) to nonhermitean ones, describing dissipative TLS. The reader should note that the use of the superadiabatic basis leads to a pre-exponential factor in Eq. (52) which is equal to one, which is identical to the case without dissipation. The result, Eq. (52), exhibits that the “dynamical” contributions follow from the adiabatic eigenvalues and their branch points, whereas the “geometrical” contributions involve  $\alpha_{\pm}(\tau)$ , only. If we parametrize for a TLS with hermitean Hamiltonian the external field components  $B_j$ , Eq. (6), as it has been done in Ref. [11], one recovers that  $F_g^{ns} = 0$  and that Eq. (53) becomes:

$$F_g^s = \int_0^{\tau_c(k)} d\tau \dot{\phi}(\tau) \cos \Theta(\tau) \quad (54)$$

in agreement with the result in Ref. [11].

### III. APPLICATION TO THE AKULIN-SCHLEICH MODEL

The AS-model is given by [19]

$$H(t) = -\frac{1}{2} [W(t)\sigma_z + \Delta\sigma_x + i\gamma(\sigma_z - \sigma_0)] \quad (55)$$

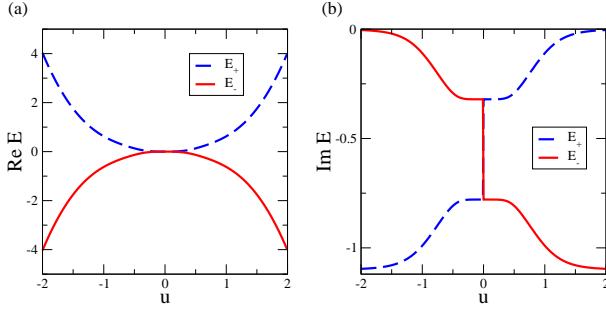


FIG. 2: Same as Fig. 1, but for  $\tilde{\gamma} = 1.1 > \tilde{\gamma}_c$

with the external field  $W(t)$ , the tunnelling matrix element  $\Delta$ , and the damping constant  $\gamma \geq 0$  of level  $|2\rangle \hat{=} |\uparrow\rangle$ .  $\sigma_0$  is the  $2 \times 2$  unit matrix. Let us introduce dimensionless quantities:

$$\tilde{w}(u) = \frac{W(t)}{\Delta}, \quad u = \frac{vt}{\Delta}, \quad \tilde{\gamma} = \frac{\gamma}{\Delta}, \quad \tilde{\epsilon} = \frac{\Delta^2}{\hbar v}. \quad (56)$$

Note that the time variable  $\tau$  of the previous section is not dimensionless. After the replacement of  $\tau$  by  $u$ , Eq. (1) takes the form of Eq. (8) with:

$$\delta = \tilde{\epsilon}^{-1}. \quad (57)$$

From Eqs. (49) and (50) it follows immediately

$$E_{\pm}(u) = \frac{1}{2} \left[ -i\tilde{\gamma} \pm \sqrt{(\tilde{w}(u) + i\tilde{\gamma})^2 + 1} \right] \quad (58)$$

$$\alpha_{\pm}(u) = -(\tilde{w}(u) + i\tilde{\gamma}) \pm \sqrt{(\tilde{w}(u) + i\tilde{\gamma})^2 + 1}, \quad (59)$$

where the branch of the square root has been chosen such that  $\sqrt{x} \geq 0$ , for  $x \geq 0$ . Fig. 1a and Fig. 1b exhibit  $\text{Re}E_{\pm}(u)$ , and  $\text{Im}E_{\pm}(u)$ , respectively, for an analytical power law sweep  $\tilde{w}(u) = u^3$  and for  $\tilde{\gamma} < 1$ . The corresponding result for  $\tilde{\gamma} > 1$  is shown in Figures 2a and 2b. In the following we will consider crossing sweeps, only. For those it is

$$\lim_{u \rightarrow \pm\infty} \tilde{w}(u) = \pm\infty. \quad (60)$$

Returning sweeps for which  $\lim_{u \rightarrow \pm\infty} \tilde{w}(u) = -\infty$  (or  $+\infty$ ) can be treated analogously. It is easy to prove that

$$E_{\pm}(u) = \frac{1}{2} \left[ \tilde{w}(u) + \frac{1}{2\tilde{w}(u)} - \frac{i\tilde{\gamma}}{2\tilde{w}^2(u)} + \mathcal{O}(\tilde{w}^{-3}(u)) \right] \quad (61)$$

for  $u \rightarrow \pm\infty$  and

$$E_{\pm}(u) = \frac{1}{2} \left[ -\tilde{w}(u) - 2i\tilde{\gamma} - \frac{1}{2\tilde{w}(u)} + \mathcal{O}(\tilde{w}^{-2}(u)) \right] \quad (62)$$

for  $u \rightarrow \mp\infty$ .

From Eqs. (61) and (48) it follows that  $F_d^{ns}$  is finite provided  $\int_u^\infty du' \tilde{w}^{-3}(u')$  exists for  $u \rightarrow \pm\infty$ . This

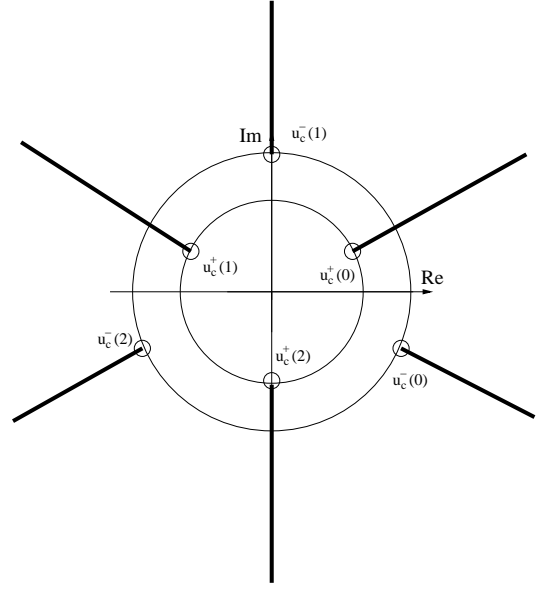


FIG. 3: Branch points (open circles)  $u_c^{\pm}(k)$  of  $E_+(u) - E_-(u)$  for a power law sweep  $\tilde{w}(u) = u^3$  and  $\tilde{\gamma} < \tilde{\gamma}_c$ . The thick solid lines are the branch cuts. The radius of the inner and outer circle is  $(1 - \tilde{\gamma})^{1/3}$  and  $(1 + \tilde{\gamma})^{1/3}$ , respectively

is fulfilled if  $\tilde{w}(u)$  decays faster than  $u^{-1/3}$ . Otherwise  $F_d^{ns} = \infty$  which makes  $P(\delta)$  to vanish. Figs. 1 and 2 demonstrate that there exists a critical value for  $\tilde{\gamma}_c$ . For  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c = 1$  we have  $\text{Re}[E_+(u) - E_-(u)] > 0$  for all  $u$  and  $\text{Im}E_{\sigma}(u)$  is continuous whereas  $\text{Re}[E_+(u) - E_-(u)]$  vanishes if  $\tilde{w}(u) = 0$  and  $\text{Im}E_{\sigma}(u)$  becomes discontinuous, provided  $E_{\pm}(u)$  are defined by Eq. (58).

The nonsingular geometrical part, Eq. (47), can be calculated without specifying the  $u$ -dependence of  $\tilde{w}$ . Substituting  $\alpha_{\pm}(u)$  and  $\tilde{\alpha}_{\pm}(u)$  from Eq. (59) into Eq. (47), both integrals in Eq. (47), become a sum of two integrals. One of them can be calculated by the introduction of a new integration variable  $\zeta = \tilde{w} + i\tilde{\gamma}$  and the other by noticing that its integrand can be rewritten as a derivative of a logarithm with respect to  $u$ . Without restricting generality we assume that  $\tilde{w}(0) = 0$ . Then we obtain with Eq. (60)

$$F_g^{ns}(\tilde{\gamma}) = 2\text{Re} \left[ \ln(i\tilde{\gamma} + \sqrt{1 - \tilde{\gamma}^2}) \right]. \quad (63)$$

The nonsingular “dynamical” and both singular contributions require the explicit  $u$ -dependence of  $\tilde{w}$ . As said above we will consider crossing sweeps only. Therefore we restrict ourselves to power law sweeps  $\tilde{w}(u) = u^n$  with  $n > 0$  and  $n$  odd.  $n$  should not be confused with the truncation number  $n$  in the previous section. Since  $\tilde{w}(-u) = -\tilde{w}(u)$  we can rewrite  $F_d^{ns}$  as follows:

$$F_d^{ns}(\tilde{\gamma}) = 2 \int_0^\infty du \left[ \tilde{\gamma} - \text{Im} \sqrt{(\tilde{w}(u) + i\tilde{\gamma})^2 + 1} \right]. \quad (64)$$

It is easy to see that

$$F_g^{ns}(0) = 0, \quad F_d^{ns}(0) = 0, \quad (65)$$

for  $\tilde{\gamma} = 0$ . Hence, the nonsingular contributions to the nonadiabatic transition probability vanish if there is no dissipation. In this case the result (52) reduces to that found by Berry [11] for hermitean Hamiltonians and for a single complex crossing point contributing to Eq. (52). What remains is the determination of the singular points  $u_c(k)$ ,  $k = 1, 2, \dots$  and the calculation of  $z_c(k)$  and  $F_g^s(k)$ . These singular points are the branch points of  $E_+(u) - E_-(u)$ . Their location depends on whether  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c$  or  $\tilde{\gamma} > \tilde{\gamma}_c = 1$ . Let us start with the *first* case  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c$ . From  $(u^n + i\tilde{\gamma})^2 + 1 = 0$ ,  $n$  odd, we find

$$u_c^\pm(k) = \pm(1 \mp \tilde{\gamma})^{1/\pi} \exp \left[ i \left( \frac{\pi}{2n} + k \frac{2\pi}{n} \right) \right] \quad (66)$$

for  $k = 0, 1, \dots, n-1$ , which are shown together with the branch cuts in Figure 3 for  $n = 3$ . From Eqs. (51) and (66) we obtain the corresponding singular points in the complex  $z$ -plane:

$$z_c^\pm(k) = \pm h_n^\pm(\tilde{\gamma}) \exp \left[ i \left( \frac{\pi}{2n} + k \frac{2\pi}{n} \right) \right] \quad (67)$$

where

$$h_n^\pm(\tilde{\gamma}) = \int_0^{(1 \mp \tilde{\gamma})^{1/\pi}} dx \sqrt{1 - (\tilde{\gamma} \pm x^n)^2}. \quad (68)$$

Since the mapping  $z(u)$  is analytic in the complex  $u$ -plane, except at the branch lines, it is conformal. Accordingly, for those  $u_c^\pm(k)$  which are in the upper  $u$ -plane the corresponding  $z_c^\pm(k)$  will be above the integration contour  $\mathcal{C}$  and therefore will contribute to  $P$  (see end of the second section). After the determination of the singular points we can proceed to calculate their “geometrical” and “dynamical” contribution to  $P$ . From Eqs. (53) and (59) it follows:

$$\begin{aligned} F_g^s(k) &= \int_0^{u_c^\pm(k)} du \frac{\dot{\alpha}_+(u) - \dot{\alpha}_-(u)}{\alpha_+(u) - \alpha_-(u)} \\ &= - \int_{\tilde{w}(0) + i\tilde{\gamma}}^{\tilde{w}(u_c^\pm(k)) + i\tilde{\gamma}} d\zeta \frac{1}{\sqrt{\zeta^2 + 1}} \\ &= -\ln(-\alpha_-(u_c^\pm(k))) + \ln(i\tilde{\gamma} + \sqrt{1 - \tilde{\gamma}^2}) \quad (69) \end{aligned}$$

Because  $(\tilde{w}(u_c^\pm(k)) + i\tilde{\gamma}) + 1 = 0$  we get from Eq. (59) that  $\alpha_-(u_c^\pm(k)) = 1$  such that

$$F_g^s(k) = \ln(i\tilde{\gamma} + \sqrt{1 - \tilde{\gamma}^2}) + i\pi \equiv F_g^s(\tilde{\gamma}). \quad (70)$$

The reader should note that  $F_g^s$  is independent on  $k$ . Consequently it can be taken in front of the sum in

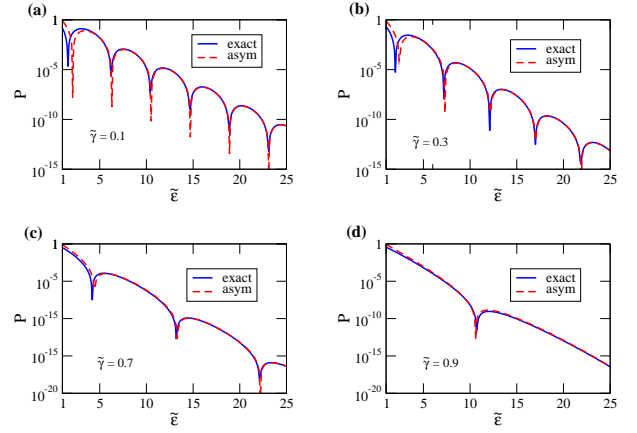


FIG. 4: Comparison of the numerical exact (solid line) and the asymptotic result, Eq. (71), (dashed line) for  $P(\tilde{\epsilon}, \tilde{\gamma})$  and a power law sweep  $\tilde{w}(u) = u^3$ . (a)  $\tilde{\gamma} = 0.1$ , (b)  $\tilde{\gamma} = 0.3$ , (c)  $\tilde{\gamma} = 0.7$  and (d)  $\tilde{\gamma} = 0.9$

Eq. (52) which yields  $\exp(2\text{Re}F_g^s)$  and just cancels the non-singular “geometrical” factor  $\exp(-2\text{Re}F_g^{ns})$ , due to Eq. (63). Therefore we find that no “geometrical” factor occurs for the AS-model. This will change if we apply an additional *time-dependent* field in the  $x$ - and  $y$ -direction. What remains is the calculation of the singular “dynamical” factor. Because we are interested in the adiabatic limit  $\delta \rightarrow 0$ , we have to take into account in Eq. (52) those singularities in the upper  $z$ -plane with smallest imaginary part. These are  $z_c^+(k=0)$  and  $z_c^+(k=(n-1)/2)$ , for which  $\text{Re}z_c^+(0) = -\text{Re}z_c^+((n-1)/2)$  and (of course)  $\text{Im}z_c^+(0) = \text{Im}z_c^+((n-1)/2)$ . Using Eq. (67) with  $k=0$  and  $k=(n-1)/2$  we obtain finally:

$$\begin{aligned} P &\cong 4 \cos^2 \left( \tilde{\epsilon} h_n^+(\tilde{\gamma}) \cos \frac{\pi}{2n} \right) \exp[-\tilde{\epsilon} F_d^{ns}(\tilde{\gamma})] \\ &\quad \times \exp[-2\tilde{\epsilon} h_n^+(\tilde{\gamma})] \sin \frac{\pi}{2n}. \quad (71) \end{aligned}$$

Let us consider linear sweeps, i.e.  $n = 1$ . Then there exists only one singularity  $u_c^+(0) = i(1 - \tilde{\gamma})$  in the upper  $u$ -plane and Eq. (52) reduces to

$$P \cong \exp \left[ -\frac{1}{\delta} [F_d^{ns} + 2\text{Im}z_c^+(0)] \right]. \quad (72)$$

The exponent can be calculated analytically by using  $u + i\tilde{\gamma}$  as an integration variable. As a consequence one finds that the  $\tilde{\gamma}$ -dependence drops out from the exponent. With  $\delta = \tilde{\epsilon}^{-1}$  one obtains

$$P \cong e^{-\epsilon}, \quad \epsilon \equiv \frac{\pi \tilde{\epsilon}}{2} = \frac{\pi \Delta^2}{2\hbar v}, \quad (73)$$

consistent with the finding in Ref. [19]. In order to check the validity of Eq. (71), we have solved numerically the time dependent Schrödinger equation in order to determine  $P$ . A comparison between the numerically exact and the asymptotic result, Eq. (71), is shown in Fig. 4

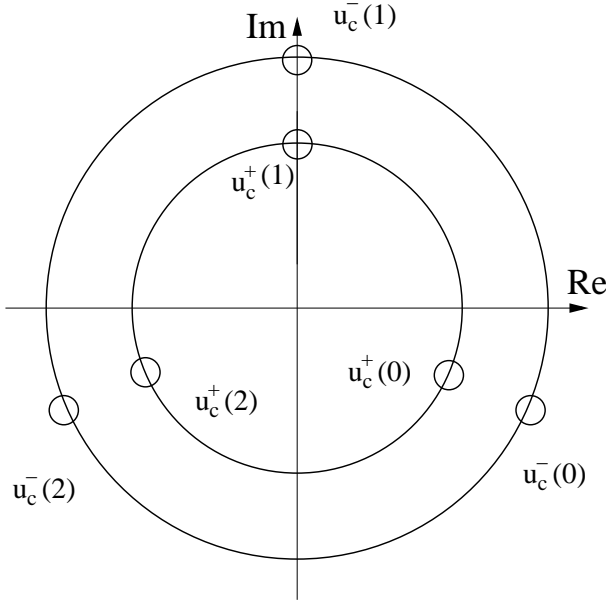


FIG. 5: Same as Fig. 3 but for  $\tilde{\gamma} > \tilde{\gamma}_c$  and without branch cuts. The radius of the inner and outer circle is  $(\tilde{\gamma} - 1)^{1/3}$  and  $(\tilde{\gamma} + 1)^{1/3}$ .

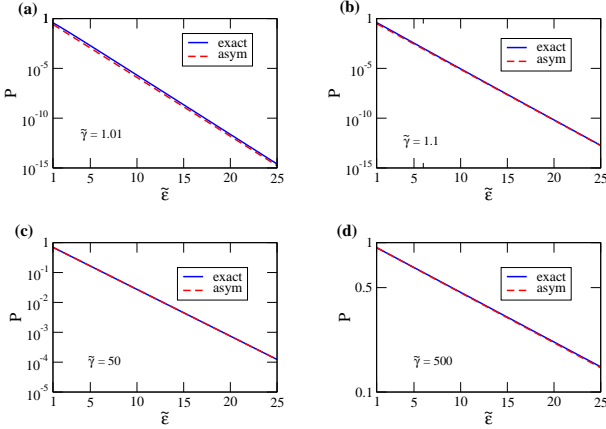


FIG. 6: Same as Fig. 4, however for  $\tilde{\gamma} > \tilde{\gamma}_c$  and with the asymptotic result, Eq. (75). (a)  $\tilde{\gamma} = 1.01$ , (b)  $\tilde{\gamma} = 1.1$ , (c)  $\tilde{\gamma} = 50$  and (d)  $\tilde{\gamma} = 500$

for  $n = 3$  and four different  $\tilde{\gamma}$ -values. We observe that the deviation between both results, e.g., for  $\tilde{\epsilon} = 5$  and  $\tilde{\gamma} = 0.3$ , is about 1.6 per cent, only. Similarly good agreement has been found for  $n > 3$ . From Eq. (71) it follows that there exist an infinite number of critical values  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$ ,  $\nu = 1, 2, 3, \dots$  at which the oscillatory prefactor in Eq. (71) vanishes. From this we can conclude that these Stückelberg oscillations proven to exist for TLS without dissipation [10] and discussed later in Refs. [9, 23] for  $\tilde{\gamma} = 0$  survive even in presence of dissipation, provided  $\tilde{\gamma} < \tilde{\gamma}_c = 1$ . Indeed, we will see below that they disappear for  $\tilde{\gamma} > \tilde{\gamma}_c$ . It is not only the survival

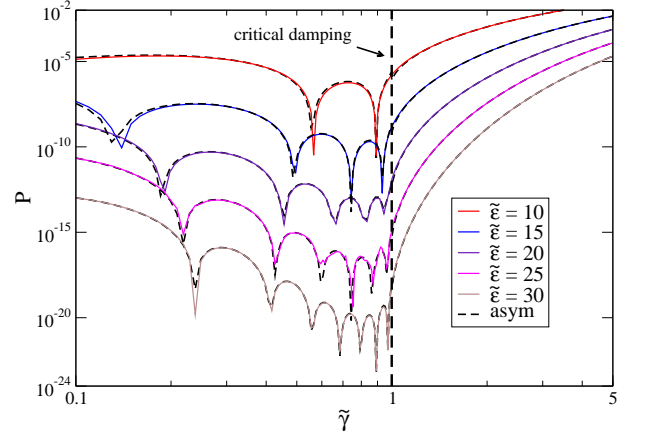


FIG. 7:  $\tilde{\gamma}$ -dependence of  $P(\tilde{\epsilon}, \tilde{\gamma})$  for  $\tilde{w}(u) = u^3$  and  $\tilde{\epsilon} = 10, 15, 20, 25, 30$  (from top to bottom). Numerical exact result (solid line) and the asymptotic one (dashed line)

of the oscillations, but also the survival of the *complete* transitions from state  $|1\rangle \hat{=} |\downarrow\rangle$  to state  $|2\rangle \hat{=} |\uparrow\rangle$  found in Refs. [9, 23] for  $\tilde{\gamma} = 0$ , as long as  $\tilde{\gamma} < \tilde{\gamma}_c$ .

Now, we turn to the *second* case  $\tilde{\gamma} > \tilde{\gamma}_c$ . For this case we find:

$$u_c^\pm(k) = -(\tilde{\gamma} \mp 1)^{1/n} \exp \left[ i \left( \frac{\pi}{2n} + k \frac{2\pi}{n} \right) \right] \quad (74)$$

for  $k = 0, 1, \dots, n-1$ , which are shown in Fig. 5 for  $n = 3$ . The main difference to the case  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c$  is that there is exactly one singular point among  $u_c^\pm(k)$  denoted by  $u_c^0$  for which  $z_c^0 = z(u_c^0)$  is on the real axis in the complex  $z$ -plane. Using the definition, Eq. (58), of  $E_\pm(u)$ , Fig. 2 demonstrates that  $E_\pm(u)$  is discontinuous on the real  $u$  axis. There seem to exist two possibilities to deal with this problem. First, after having chosen the branch cuts in the complex  $u$ -plane one has to deform the integration contour along the real  $u$ -axis such that  $u = 0$  is above that contour and that no branch cut is crossed. This kind of reasoning was used by Moyer in Ref. [20]. Second, one could define  $E_\pm(u)$  such that they are analytic in a strip around the real  $u$ -axis. This can be done by interchanging  $E_+(u)$  and  $E_-(u)$  for  $u \leq 0$ . This has the consequence that the contour  $z(u)$  for  $u$  real is in the right complex  $z$ -plane, starting e.g. above the positive real axis for  $u = -\infty$ , going through  $z = 0$  for  $u = 0$  and then continuing below the positive real axis for  $u \rightarrow +\infty$ . This contour would enclose  $z_0$  if  $\text{Re} z_0 > 0$ . Whether it can be closed such that the closure does not make a contribution is not obvious. Since we are not sure how to solve this problem in a rigorous manner, we have assumed that  $z_0$  is the leading contribution to  $P$ , Eq. (52), for  $\delta \rightarrow 0$ . Since  $|e^{iz_c^0/\delta}| = 1$  and due to the absence of a “geometrical” contribution we obtain:

$$P \cong \exp[-\tilde{\epsilon} F_d^{ns}(\tilde{\gamma})], \quad (75)$$

with  $F_d^{ns}(\tilde{\gamma})$  given by Eq. (64). A comparison between the  $\tilde{\epsilon}$ -dependence of the numerically exact and the



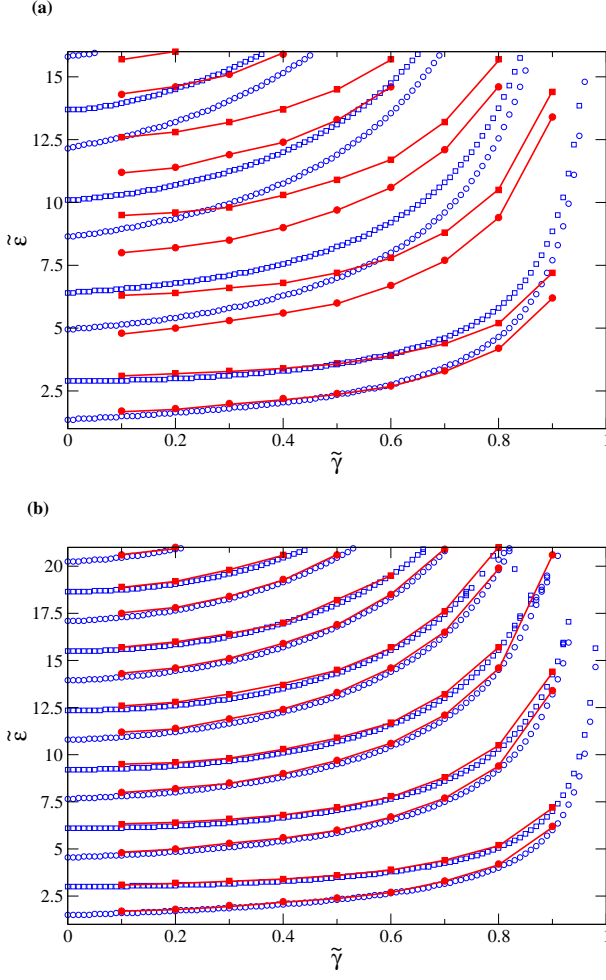


FIG. 8: Comparison of the critical values  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$  for (a)  $\tilde{w}(u) = u^5$  and (b)  $\tilde{w}(u) = u^{51}$ . The numerically exact result is shown by the open circles and the result obtained for the oscillator model is depicted by the full circles. The solid lines are a guide for the eye.

asymptotic result, Eq. (75), is presented in Fig. 6. Again we find a very good agreement already for  $\tilde{\epsilon} \geq 1$ . This strongly supports the correctness of our assumption that  $z_0$  is the most important singularity. Eq. (75) reveals that the Stückelberg oscillations as function of  $\tilde{\epsilon}$  have disappeared. We stress that both asymptotic results, Eq. (71) and (75), are valid for all  $\tilde{\gamma}$  with  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c$  and for all  $\tilde{\gamma}$  larger than  $\tilde{\gamma}_c$ , respectively, provided  $\tilde{\epsilon}$  is large enough. This is demonstrated in Fig. 7 for different  $\tilde{\epsilon}$ .

#### IV. INTERPRETATION BY A DAMPED HARMONIC OSCILLATOR

In this section we will give an intuitive explanation of the Stückelberg oscillations and will present an approximate calculation for the critical values  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$  for power law crossing sweeps  $\tilde{w}(u) = u^n$ ,  $n$  odd. Close to

the resonance at  $u = 0$  we may neglect  $\tilde{w}(u)$ . Then the time dependent Schrödinger equation for the amplitude of state  $|1\rangle$

$$\tilde{c}_1(u) = c_1(u) \exp \left[ i \int_{-\infty}^u du' \tilde{w}(u') \right] \quad (76)$$

becomes

$$\ddot{\tilde{c}}_1 + 2\mu\dot{\tilde{c}}_1(u) + \omega_0^2\tilde{c}_1(u) \cong 0 \quad (77)$$

with:

$$\mu = \frac{\tilde{\epsilon}\tilde{\gamma}}{2}, \quad \omega_0 = \frac{\tilde{\epsilon}}{2}. \quad (78)$$

Let  $t_{\text{trans}}$  be the Landau-Zener transition time. In the adiabatic limit it is well-known that  $t_{\text{trans}} = \Delta/v$ . Eq. (56) yields  $u_{\text{trans}} = 1$ . Therefore we will require as initial conditions:

$$\begin{aligned} \tilde{c}_1(-u_{\text{trans}} = -1) &= 1 \\ \dot{\tilde{c}}_1(-u_{\text{trans}} = -1) &= 0. \end{aligned} \quad (79)$$

Eq. (77) is the equation of motion for a damped harmonic oscillator which can easily be solved. The special solutions are  $\exp[i\omega_{\pm}(\tilde{\epsilon}, \tilde{\gamma})u]$  with

$$\omega(\tilde{\epsilon}, \tilde{\gamma}) = \frac{\tilde{\epsilon}}{2} \left[ i\tilde{\gamma} \pm \sqrt{1 - \tilde{\gamma}^2} \right]. \quad (80)$$

This result makes obvious the existence of a critical damping  $\tilde{\gamma}_c = 1$ . For  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c$  and  $\tilde{\gamma} < \tilde{\gamma}_c$  the oscillator is underdamped and overdamped, respectively. This qualitative different behavior is the origin of the different  $\tilde{\epsilon}$ -dependence of  $P$  for  $0 \leq \tilde{\gamma} < \tilde{\gamma}_c$  and  $\tilde{\gamma} < \tilde{\gamma}_c$ , found in the third section. This relationship can be deepened more by calculating  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$ . Having solved Eq. (77) with initial conditions, Eq. (79) we approximate  $P$  by:

$$P \cong |c_1(+u_{\text{trans}}) = +1|^2 = |\tilde{c}_1(+u_{\text{trans}} = +1)|^2. \quad (81)$$

The zeros (with respect to  $\tilde{\epsilon}$ ) of  $P$  yield  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$ . A numerical solution of the corresponding transcendental equation leads to the results shown in Figure 8 for  $\tilde{w}(u) = u^n$  with  $n = 5$  and  $n = 51$  and  $\tilde{\gamma} < \tilde{\gamma}_c$ . Figure 8 also contains the result from a numerically exact solution of the time dependent Schrödinger equation. Comparing both results we observe that the agreement for  $n = 5$  is qualitatively good, but quantitatively less satisfactory. However, increasing  $n$  more and more leads even to a rather good quantitative agreement, as can be seen for  $n = 51$ . This behavior is easily understood, since  $\tilde{w}(u)$  within the transition range  $(-1, 1)$  becomes practically zero for  $n$  large enough. Figure 8 also demonstrates that  $\tilde{\epsilon}_c^{(\nu)}$  increases monotonically with  $\tilde{\gamma}$  which is related to the decrease of  $\text{Re}w(\tilde{\epsilon}, \tilde{\gamma})$  for increasing  $\tilde{\gamma}$ . The oscillator model can also be used to determine a lower bound for  $\tilde{\epsilon}_c^{(1)}(\tilde{\gamma} = 0)$ . For  $u_{\text{trans}} = 1$  one gets

$$\tilde{\epsilon}_c^{(1)}(\tilde{\gamma} = 0) \geq \frac{\pi}{2} \quad (82)$$

such that  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma}) \geq \tilde{\epsilon}_c^{(1)}(\tilde{\gamma}) > \tilde{\epsilon}_c^{(1)}(\tilde{\gamma} = 0) \geq \pi/2$ , for all  $\tilde{\gamma}$ . It is interesting that the lower bound (82) for  $\tilde{\epsilon}$  is similar to that obtained from the *inverse* Landau-Zener problem [25]. There, the  $t$ -dependent survival probability  $P(t; \tilde{\epsilon})$  is given and  $W(t; \tilde{\epsilon})$  is determined analytically from  $P(t; \tilde{\epsilon})$ . If  $P(t; \tilde{\epsilon}) = P(t; \tilde{\epsilon}u)$ , with  $u$  and  $\tilde{\epsilon}$  from Eq. (56), varies from one (for  $t = -\infty$ ) to zero (for  $t = +\infty$ ), it is found that a solution  $W(t; \tilde{\epsilon})$  of the inverse problem only exists, if

$$\tilde{\epsilon} > 1. \quad (83)$$

The latter inequality, as well as inequality (82) implies that the ratio  $t_{\text{trans}}/t_{\text{tunnel}}$  of the transit time  $t_{\text{trans}} = \Delta/v$  and the time period of coherent tunneling  $t_{\text{tunnel}} = \hbar/v$ , which equals  $\tilde{\epsilon}$ , is of order one. It is obvious that *complete* transitions can not occur if  $t_{\text{trans}}$  is too small compared to  $t_{\text{tunnel}}$ , i.e. for  $\tilde{\epsilon} \ll 1$ . In that case the quantum system does not have time enough to tunnel from the initial state  $|1\rangle$  to state  $|2\rangle$ .

## V. SUMMARY AND CONCLUSIONS

Our main focus has been on the derivation of the non-adiabatic transition probability  $P(\tilde{\epsilon})$  for a dissipative two-level system modelled by a *general* non-hermitean Hamiltonian, depending analytically on time. Following for the hermitean case Berry's approach by use of a superadiabatic basis we have found a generalization of the DDP-formula. Besides a "geometrical" and a "dynamical" factor, completely determined by the crossing points in the complex time plane, we also have found a non-universal "geometrical" and "dynamical" contribution to  $P$ . The latter require the knowledge of the Hamiltonian's full time dependence and are identical to zero in the absence of dissipation. Without specification of the TLS-Hamiltonian, we have shown that both "geometrical" contributions can be expressed by  $\alpha_{\pm}(u)$ , the ratio of the components of each adiabatic states  $|u_{0,\pm}(u)\rangle$  in the basis  $|\nu\rangle$ ,  $\nu = 1, 2$ , and both "dynamical" ones by the adiabatic eigenvalues  $E_{\pm}(u)$ , only. In this respect our result for  $P(\tilde{\epsilon})$  is independent of a special parametrization of the Hamiltonian matrix. Although the result in Ref. [20] is not in such an explicit form like Eq. (46) the existence of this nonsingular "dynamical" contribution has already been stated there. However, the nonsingular "geometrical" part, Eq. (47), has not been found in that paper.

As a physical application we have studied the AS-model [19]. This model describes a dissipative TLS where the initial upper level is damped. In [19] it has been shown that the probability  $P$  for a linear time dependence of the bias does not depend on the damping constant  $\tilde{\gamma}$  for all  $\tilde{\epsilon}$ . Our results demonstrate that this is not generic. For instance, nonlinear power law crossing sweeps generate a  $\tilde{\gamma}$ -dependence of  $P$ . For such sweeps a critical value  $\tilde{\gamma}_c = 1$  exists. Below  $\tilde{\gamma}_c$  the non-adiabatic transition probability oscillates and vanishes at critical values  $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$ , and for

$\tilde{\gamma} > \tilde{\gamma}_c$  the oscillations are absent. Hence, the existence of complete transitions at an infinite set of critical sweep rates still holds for all  $\tilde{\gamma}$  below  $\tilde{\gamma}_c$ . In the section IV we have shown how the oscillations and their disappearance for  $\tilde{\gamma} > \tilde{\gamma}_c$  can be qualitatively explained by a damped harmonic oscillator. For power law sweeps with rather large exponent, e.g.  $n = 50$ , this description becomes even quantitatively correct. No doubt, it would be interesting to study a microscopic model of a TLS coupled to phonons, e.g. a spin-boson-Hamiltonian as in Ref. [13], in order to check whether the  $\tilde{\epsilon}$ -dependence of  $P$  exhibits oscillations for power law sweep with  $n > 1$  and small enough spin-phonon coupling. Another question concerns the interaction between the TLS which have been completely neglected in our present work. That they can play a crucial role was shown recently [26]. Whether the oscillations still exist in the presence of interactions between the TLS is not obvious.

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## Appendix

In this appendix we will describe how the asymptotic result, Eq. (52), has been derived from (46). Although we follow Berry's approach [11, 22] we repeat the most important steps since the non-hermitean property of  $H$  does not allow the simple parametrization used in Ref. [11] and is not of the form of Eq. (84) or Eq. (87) of Ref. [22]. Nevertheless we will recover the same universal recursion relation for the coefficients  $a_m^-(\tau)$  as found by Berry [22]. In order to show how Eq. (52) can be obtained from Eq. (46) we have to calculate the three pre-exponential factors  $E_+(\tau) - E_-(\tau)$ ,  $[\alpha_+(\tau) - \alpha_-(\tau)]/\dot{\alpha}_+(\tau)$  and  $\dot{a}_{n+1}^-(\tau)$  in Eq. (46). We assume that the Hamiltonian  $H(\tau)$  is analytic in  $\tau$ . Let  $\tau_c$  be one of the branch points of  $E_+(\tau) - E_-(\tau)$ . Close to  $\tau_c$  we get:

$$E_+(\tau) - E_-(\tau) \cong c(\tau - \tau_c)^{1/2} \quad (84)$$

with  $c$  a constant, depending on  $\tau_c$ . Eq. (51) implies

$$z - z_c \cong \frac{2}{3}c(\tau - \tau_c)^{3/2}, \quad (85)$$

where  $z_c = z(\tau_c)$ . In the adiabatic limit  $\delta \rightarrow 0$  the main contribution to the integral (2. line of Eq. (46)) comes from the singular points  $\tau_c$  and  $z_c$ , respectively. Consequently we have to calculate the pre-exponential factors (2. line of Eq. (46)) close to the singularities, only. Let us start with  $[\alpha_+(\tau) - \alpha_-(\tau)]/\dot{\alpha}_+(\tau)$ . Using Eq. (50) it follows with  $\alpha_{\pm}(z) = \alpha_{\pm}(\tau(z))$  close to  $z_c$

$$[\alpha_+(z) - \alpha_-(z)]/\alpha'_+(z) \cong 6(z - z_c), \quad (86)$$

where ' denotes derivative with respect to  $z$ . Note that  $H_{11}, H_{12}$  and  $H_{22}$  do not enter in Eq. (86). The calculation of  $\dot{a}_{n+1}^-(\tau)$  is more evolved. As a first step we eliminate  $\dot{b}_{m-1}^-(\tau)$ ,  $b_{m-1}^-(\tau)$  and  $b_m^-(\tau)$  from Eqs. (23), (24) which yields a recursion relation for  $a_m^-(\tau)$ :

$$\dot{a}_m^-(\tau) = \frac{i}{E_+(\tau) - E_-(\tau)} \left[ \ddot{a}_{m-1}^-(\tau) - \frac{\dot{\kappa}_-(\tau)}{\kappa_-(\tau)} \dot{a}_{m-1}^-(\tau) - \kappa_-(\tau) \kappa_+(\tau) a_{m-1}^-(\tau) \right]. \quad (87)$$

Next we calculate the various terms close to  $\tau_c$ . From Eqs. (30) and (50) we get:

$$\frac{\dot{\kappa}_-(\tau)}{\kappa_-(\tau)} \cong (\tau - \tau_c)^{-1} \quad (88)$$

and

$$\kappa_-(\tau) \kappa_+(\tau) \cong \frac{1}{16} (\tau - \tau_c)^{-2}. \quad (89)$$

Expressing the  $\tau$ -derivatives of  $a_m^-$  and  $a_{m-1}^-$  by derivatives with respect to  $z$ :

$$\dot{a}_m^-(\tau) \cong c(\tau - \tau_c)^{1/2} a_m'^-(z) \quad (90)$$

and

$$\ddot{a}_m^-(\tau) \cong c^2(\tau - \tau_c) a_m''^-(z) + \frac{c}{2} (\tau - \tau_c)^{-1/2} a_m'^-(z), \quad (91)$$

where  $dz/d\tau = E_+(\tau) - E_-(\tau)$  and (84) was used, we get from Eq. (87) with Eq. (88), (89):

$$a_m''^-(z) \cong (-i) \left[ \frac{a_{m-1}^-(z)}{36(z - z_c)^2} - \frac{a_{m-1}'^-(z)}{(z - z_c)} - a_{m-1}''^-(z) \right] \quad (92)$$

with initial condition (cf. Eq. (28)):

$$a_0^-(z) \equiv 1. \quad (93)$$

The recursion relation is identical to Eq. (30) in Ref. [22], except the different sign in front of the square bracket. The sign change is irrelevant. The exact solution of Eq. (92), (93) can be taken from Ref. [22]:

$$a_m^-(z) \cong B_m (z - z_c)^{-m} \quad (94)$$

with

$$B_m = i^m \frac{(m - \frac{7}{6})! (m - \frac{5}{6})!}{m! (-\frac{7}{6})! (-\frac{5}{6})!}. \quad (95)$$

Then we get from Eq. (46) with (84) - (86) and (94), (95)

$$\begin{aligned} & \int_{-\infty}^{\infty} d\tau \dot{a}_{n+1}^-(\tau) \frac{\alpha_-(\tau) - \alpha_+(\tau)}{\dot{\alpha}_+(\tau)} [E_+(\tau) - E_-(\tau)] I(\tau) \\ &= \int_{\mathcal{C}} dz a_{n+1}'^-(z) \frac{\alpha_+(z) - \alpha_-(z)}{\alpha_+'(z)} I(z) \\ &= -6(n+1) B_{n+1} \sum_k \int_{\mathcal{C}} dz \frac{1}{(z - z_c(k))^{n+1}} I(z) \\ &= -6(n+1) 2\pi i \left( \frac{i}{\delta} \right)^n B_{n+1} \sum_k I(z_c(k)), \end{aligned} \quad (96)$$

where the sum over  $k$  is restricted to all singular points  $z_c(k)$  above the contour  $\mathcal{C} = \{z = z(\tau) | -\infty \leq \tau \leq \infty\}$ . Since

$$-6 \cdot 2\pi(n+1) B_{n+1}/n! \longrightarrow i^{n+1}, \quad n \rightarrow \infty, \quad (97)$$

the prefactor in front of  $\sum_k$  in Eq. (96) equals  $(-1)^{n+1}$ .

Substituting (96) into Eq. (46)  $\delta^n$  cancels and one obtains the result Eq. (52).

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